



ProHits MS Data Management

User manual - demo

Version demo 1, prepared on Feb 09, 2010 by Anne-Claude Gingras, (earlier versions prepared with the help of Frank Liu, JP Zhang, Brian Raught, Brett Larsen, Karen Colwill, Zhen Lin and Lisa D'Ambrosio).

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Using the "MS Data Management" module

Once you have selected the MS Data Management module from the ProHits access page and have logged in, the following screen will appear.

At the top of the page (left), you will find the tabs "Home", "Storage" and "Auto Search" that allow you to navigate between the storage and the search areas of the MS Data Management Module. On the left is a link to the Analyst module that can be accessed from every page of the MS Data Management module.

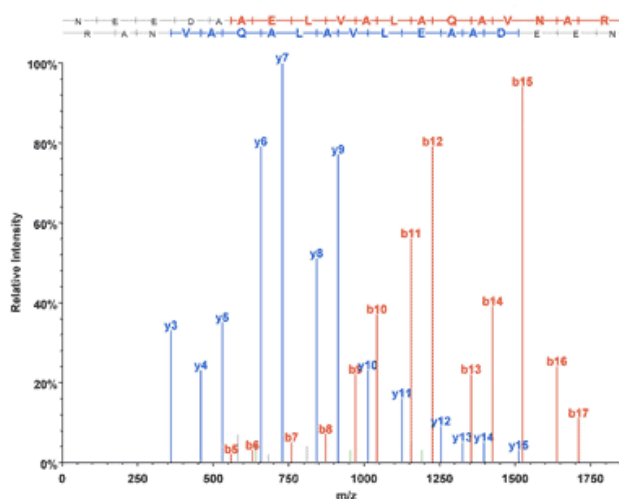


Overview

Welcome to ProHits

ProHits is an open source software tool designed to help scientists manage, search and analyze mass spectrometry data.

MS Data Management allows you to store raw mass spectrometry data from multiple instruments, and to initiate database searches using the commercial Mascot search engine (licence from Matrix Science is necessary) and/or the free Open Source search engine X!Tandem. Search results can be further analyzed using the TransProteomic Pipeline (TPP, an Open Source software suite), and viewed directly within the MS Data Management module. Alternatively, search engine (and/or TPP) results can be transferred (parsed) into a bait-centric relational database, the **Analyst** module.



The **Storage** section allows you to monitor the transfer of data from each of the acquisition computers to the ProHits backup system. It also allows you to search, browse and download files, convert RAW files to other formats, and manually upload RAW data.

The **Auto Search** section allows you to perform database searching on specified files using user-defined search engines and parameters, to explore the results, and to transfer search results to the Analyst module. It also allows for database searches to be pre-scheduled for data files that will be acquired at a later time.

The "Storage" section allows you to monitor the transfer of the data from each of the acquisition computers to the ProHits backup system. It also allows you to search and browse and download backed up files, convert RAW files to other formats, and manually upload RAW data.

The "Auto Search" section allows you to perform and schedule database search tasks on specified files using user-defined search engines and parameters, to explore the results and to link search results to the experimental information in the Analyst module.

Storage

⇒ Select the "Storage" tab

ProHits manages the backup and storage of data files in an instrument-dependent manner. The left of this screen provides links to all available instruments in the mass spectrometry facility (also shown as pictures). Here, you can also view the Backup log. This page also specifies the location of the database and data storage. The central part of the page details the status of each of the connections. A green arrow indicates a functional connection while a broken red arrow denotes a broken connection.

Note that this example is for the Samuel Lunenfeld Research Institute facility; the demo version lists a single instrument (LTQ_demo). For the purpose of this user manual, we will toggle between the demo version and the live site at the Samuel Lunenfeld Research Institute.

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Protein High-throughput Solution

Home Storage Auto Search Help Analyst Logout

Raw Data Storage

The storage of Prohits is designed to automatically perform data collection and management for mass spectrometry. All MS raw data files will be saved to the Prohits computer (192.197.250.146 : /export/home0/) and a MYSQL database 192.197.250.119 : prohits_manager will store the data information. This page will check all connections between Prohits and mass spectrometry computers. If there are any broken connections →, please notify Prohits administrator.

Storage Database Computer:
IP address
Storage Database Name: prohits_manager

Storage Computer:
IP address
Storage Folder: /export/home0/

4000QTRAP
LTQ
LCQtrap
LTQ1
LTQACG
LTQMT
LTQXL
Nanospray
ORBITRAP
QSTARELITE
QstarOMaldi
Qtrap

Backup Log
August 2008
Go Today

S	M	T	W	Th	F	S
					1	2
3	4	5	6	7	8	9
10	11	12	13	14	15	16
17	18	19	20	21	22	23
24	25	26	27	28	29	30
31						

04 Aug 2008

• Prohits lost connection with 4000QTRAP data folder.
The source directory is empty.

This links to individual instruments backed up on Prohits in your facility

Select to monitor file transfer from your acquisition computer to Prohits and view the log for the RAW file converters and the RAW file merge functions

Location of storage; this is set-up by your administrator

Status notification. Successful links are shown by green arrows. When Prohits is unable to backup data from one mass spectrometer, an orange broken arrow will appear. You will also see a note appearing at the bottom of the page detailing the problem..

Selecting instruments and folders

The files backup organization mirrors the set-up on each acquisition computer (the computer linked to the MS instrument). Subfolders are allowed on the acquisition computer. Selecting the instrument will open a new page allowing you to browse files and projects. In this demo version, only one instrument (LTQ_demo) is available.

⇒ **Select an instrument (LTQ_demo) by clicking on a link on the left of the page**

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LTQ DEMO

Fetch Raw File

Raw File Status.

Backup Log

February 2010

Go Today

LTQ_DEMO raw data

Backup File Now Upload Raw Files

Total : 3 (1 Page) 1

Browse Project: All Go

ID	[Project ID] Name	Type	Date	Search Task	Options
21	3 Demo_Human_GelFree_P3	dir	2010-01-06 00:00:00	5	
3	2 YST_GelFree_P2	dir	2008-07-15 16:27:14	6	
1	1 20030205_YDP00155_A1_P1	dir	2008-07-15 16:18:53	7	

At the bottom of the page, the folders associated to this instrument are listed (along a unique identifier assigned by ProHits). Folders are associated to individual "Analyst" projects defined in the Admin Office. Note that adding as a suffix to the "Demo_Human_GelFree" folder name "_P3" enables the creation of Autolinks (as will be discussed later).

The Search Task column allows you to navigate to the search results page(s) associated with files in this folder. In the Options column, clicking will open the folder, while selecting will download the files associated to this folder on your local computer.

ProHits automatically backs up any new files from the acquisition computer at a time specified by the administrator.

The user may also initiate manual back up and by clicking [Backup File Now] (towards the top of the page). Please note that to prevent file corruption, ProHits has a timed delay for file transfer (delay specified by administrator – we use 2.5 hours after last modifications).

To upload raw files from an instrument not connected to the ProHits backup system, select [Upload Raw Files] and navigate through options. This function can also be used to upload converted files to be searched in ProHits.

⇒ Select a folder (Demo_Human_GelFree_P3) to open

In addition to the files located on the acquisition computer, the selected folder will also contain any files that you have converted from original raw file to other formats, and any file types stored on the acquisition computer (e.g. .doc, .xls, etc.). This folder will also contain any file manually uploaded on the previous page. Here, we show the raw file 9_MEPCE_pelletB.RAW (acquired on a Thermo LTQ instrument) already converted to .mzXML (for searches using X!Tandem) and .mgf (for Mascot searches).

The screenshot shows the ProHits MS Data Management interface. The top navigation bar includes Home, Storage, and Auto Search. The left sidebar shows a tree view with LTQ_DEMO selected. The main content area displays 'LTQ_DEMO raw data' with a list of files. The 'Convert' column has checkboxes for each file. The 'Download' column has download icons. The 'Convert' button is highlighted.

ID	File Name	Size	Project Bait sample	Date	Search Task	Download	Convert
23	9_MEPCE_pelletB.RAW	180,071		2010-01-06 00:00:00	5		<input type="checkbox"/>
34	9_MEPCE_pelletB.mzXML	239,997		2010-01-07 15:43:30			<input type="checkbox"/>
35	9_MEPCE_pelletB.mgf	435,683		2010-01-07 16:16:23			<input type="checkbox"/>

Data file conversion

ProHits can automatically convert Thermo RAW files to the database search engine preferred file types as part of the AutoSearch pipeline. Alternatively, RAW files can easily be converted here. To convert a RAW file to mgf, mzXML or dta format, choose the desired files by clicking the boxes in the "Convert" column, select the desired format (and conversion parameters if available) and hit "Convert". If you select conversion to either .mgf or .dta files, you can combine (or merge) several files. Selecting either of these formats for conversion expands the dialog box; selecting [merge files] allows you to manually select the individual files to be merged in the final file and to give a new name to the merged file. This option is especially useful to combine files from fractionation of the same sample (e.g. gel bands from the same lane).

The screenshot shows the ProHits interface with the 'Convert Selected file to' dropdown set to 'DTA'. The 'Merge files' checkbox is checked. The 'Xcalibur Parameters' field contains '-B300 -T5000 -M1 -S1'. A modal dialog box titled 'Type merged file name' is open, with a text input field and 'Convert' and 'Cancel' buttons.

Note that at the present time the publically released version of ProHits can only convert data from Thermo instruments. Please refer to <http://tools.proteomecenter.org/wiki/index.php?title=Formats:mzXML>, <http://psidev.info/index.php?q=node/257>, or <http://proteowizard.sourceforge.net/> for converters for additional instruments proprietary formats.

Linking files to the Analyst module

As mentioned in the general introduction, RAW files located in the Data Management module can be linked to Baits>Experiments>Samples defined in the Analyst module and the Search Results can be transferred (parsed) from the Data Management module to the Analyst module.

The chain link icons in each table of the Data Management module indicate the linking status:



(broken white chain link) indicates that the file is not linked to any sample in the Analyst module,



(intact yellow chain) indicates that a link to a sample in the Analyst module has been manually created,



(intact green chain) indicates that a link has been created automatically (also called "Autolink").

⇒ To create manual links, click in the "project Bait/sample" column.

This opens up a new dialog box allowing you to select the desired Project, Bait, and Sample. Upon closing the box, the yellow chain link icon

will appear.

Creating automatic links requires interfacing with the Analyst module and using a standardized naming scheme. This will be described in a separate section.

Creation of New Baits and Samples will be described in the instructions for the Analyst module module.

Link Raw file to Prohits Sample

Raw file information

Machine Name: LTQ
Raw File: Demo_Human_GelFree_P3 / 16_FLAG_alone_pelletC.RAW
Folder Project: Demo Human Gel Free

Link to Experiment Sample

☐ Gel ☒ Gel Free

Project Name: (3) Demo Human Gel Free [new]

Bait: (10) FLAG_alone [new]

Experiment: (12) FLAG_alone_pelletC [new]

Gel: Gel Free

Sample: (16) FLAG_alone_pelletC [new]

Submit Close

This completes the overview of the "Storage" part of the Data Management module of ProHits. In the next section, we will navigate through the searching and parsing functions.

Using AutoSearch for database searching

⇒ **Select the "AutoSearch" tab at the top of the page**

This view displays all the search engines and other tools which have been linked to your ProHits database in the top portion of the page. As with the link to different mass spectrometers in the Storage area, successful links to search engines are indicated by green arrows and broken links by a broken orange arrow.

You can modify the general search parameters from this page; you will also be able to modify search parameters when initiating searches. ProHits simply employs the standard interfaces provided by the search engines and allows you to create several standard search parameters sets.

Parameter Setup
ProHits monitors connections to the search engines. Broken connections are indicated by a broken red arrow.

Storage Computer: 192.197.251.36
Storage Folder: /mnt/storage1/

Xcalibur Parameters (RawConverter)
Convert Finnigan Xcalibur RAW file to peak lists.
(http://10.197.104.18/RawConverter)

Mascot Parameters
Create or modify Mascot search parameter set.
(http://192.197.250.115/mascot)

The GPM Parameters
Create or modify the GPM search parameter set.
(http://thegpm.mshni.on.ca/tandem/thegpm_tandem.html)

The TPP Parameters
Create or modify the TPP parameter set.
(v4.0 JETSTREAM rev 2, Build 200901301833 (linux))

Tasks and Results

LTQ_DEMO

- Setup new task
- View tasks
- Browse search results by folder
- Parse search results to ProHits/Analyst

The bottom part of the page allows you to access individual instruments for search purposes, by simply clicking on the links or on the instruments.

⇒ **Select an instrument for searching (for this tutorial, we will select LTQ_Demo)**

The entry page lists all of the search tasks that were performed for files collected on a given instrument. A given task may be applied to several files not necessarily located within the same subfolder or in the same format. We will return to this list later after we have created a New Task.

The table lists the current Tasks. To view the search parameters and a list of the searched files, press . To view the search results, press: (Results details).

The left menu bar allows you to add or manage Tasks, as well as to view the logs.

LTQ_DEMO Search Tasks

Task ID	Analyst PlateID	Project	Task Name	Status	Task Detail	Result Detail
7	1	1	Gel_based demo search	Finished		
6	0	2	yeast_demo_search	Finished		
5		3	Demo_human	Finished		
1	1	1	demo search	Finished		

Total : 4 (1 Page) 1

Left Menu Bar:

- LTQ_DEMO Search Tasks
- LTQ_DEMO New Task
- LTQ_DEMO Task Finder
- Running Task Status
- View Search Log
- View TPP Log
- View Parser Log

⇒ Select "LTQ_Demo New Task"

This opens up a new page. Enter a Task Name of your choice, select the search engine(s) and parameter set(s) to be utilized (these can be edited). If needed, an automatic conversion of RAW files to the mgf format used by Mascot or the mzXML format used by X!Tandem can be applied. The search can be initiated manually and immediately ("Start Now"), or automatically as files are added every X hours (see below). You have an option of automatically running the TPP statistical software tools on the search results. If you choose to do so, select the "Run TPP" box. Note that you can also run the TPP tools after you get the search results. (Running TPP manually post-acquisition is a more flexible option, because it allows you to combine several files into a single TPP analysis).

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Home Storage **Auto Search** Help Analyst Logout

LTQ Search Task

Task Name:

Folder ID Folder Name Project

Search Engine Parameter Set
Choose either or both search engines.
Mascot ☒ demo_human Edit
The GPM ☐ human Edit

Run TPP ☐
TPP also can be set to run after the search task is finished in search results page.
TPP Name
TPP Parameter set Edit

Xcalibur Parameter
Parameters required for converting LTQ raw file to mgf file for Mascot:
-B300 -T5000 -I10 -S1 -G1 -M0.1 Edit

Search schedule
If you have a running task. This task will be in the task queue.
☐ Start Now
☐ Start Every 12 Hour

Data Files (total: 0)
Automatically add ☐ files
• Check the box if you want to auto-add newly created files to this task from the folder/plate.
[Folder ID] / File Name

Mascot Parameters
Create or modify Mascot search parameter set

Your name: frank liu Email: gliu@mshri.on.ca

Search title: demo human

Database: Human_RefseqV33

Taxonomy: All entries

Enzyme: Trypsin Allow up to: 1 missed cleavages

Fixed modifications: Acetyl (K), Acetyl (N-term), Acetyl (Protein N-term), Amidated (C-term), Amidated (Protein C-term)

Variable modifications: Cation:Na (C-term), Cation:Na (DE), Deamidated (NQ), Dehydrated (N-term C), Dehydro (C)

Quantitation: None

Peptide tol.: 3 Da # ¹³C 0 MS/MS tol.: 0.6 Da

Peptide charge: 2+ and 3+ Monoisotopic ☒ Average ☐

Data format: Mascot generic Precursor: m/z

Instrument: ESI-TRAP Error tolerant: ☐

Decoy: ☐ Report top: 200 hits

Parameter Set New Set ☐ Modify Set ☒ Set by: Prohits Administrator Set date: 2010-01-06
Set name: demo_human for Project: Demo Human Gel Free

Save Reset Close

06 Jan 2010

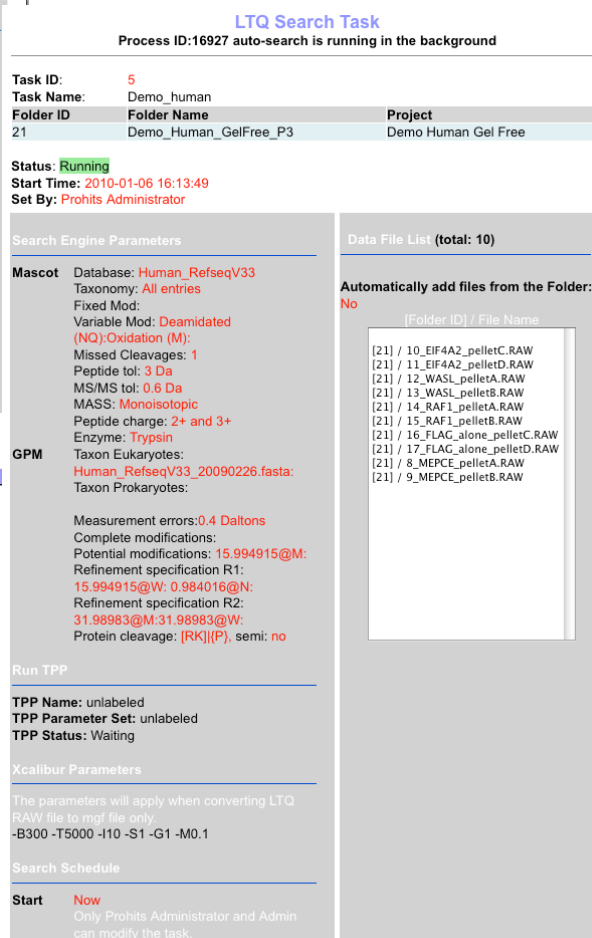
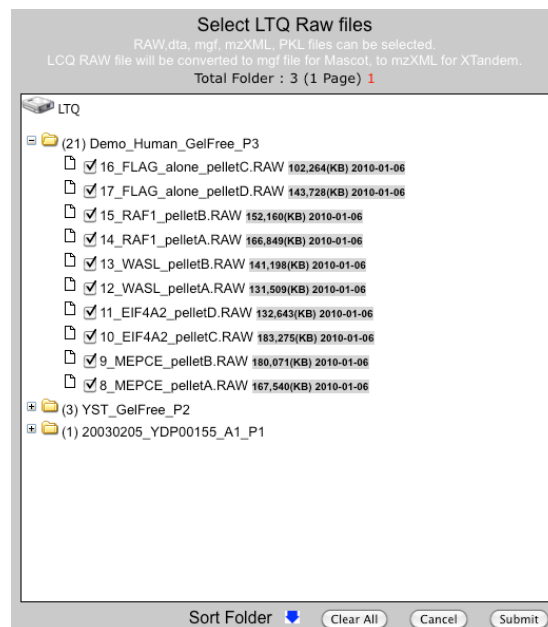
Manually initiate searches

⇒ To manually initiate a search, select the “Start Now” option, and click the “Add Files” button located on the bottom right

This will open the folders for the specified instrument, allowing you to select as many files as desired for searching.

Each user can only have one running task per machine; additional tasks (unlimited number) will be placed in a queue. The search will automatically initiate (in the order they were queued) once the initial searches are completed.

Once all parameters are selected, and the files transferred, click the “Run Task” button at the bottom of the screen.



The task will now be running, and the search parameters will be locked. Tip: instead of creating a new search task for each file you analyze using the same search parameters, use the “Modify Task” option at the bottom of the page: this will group all your searches within the same search task folder, making it easier to retrieve, and will also ensure that the same search parameters are used for each file. Clicking [Modify Task] allows you to add files to be searched with the same parameters, but not to change the search parameters. To research the same raw files with different search parameters, a New Task must be created.

Automatically initiate searches

For some high-throughput projects, users may want to **automatically initiate searches** on every new file added to the folder(s) that are initially selected for the search. Before you can select to automatically add files and search them, you have to point to at least one file in a folder manually, as indicated above. By selecting the "Start every X hours" (left hand side), and "Automatically Add Files" (right side) options, every file of the selected format subsequently acquired within the same folder(s) or subfolder(s) will be automatically searched using the same parameters.

Search Task view

⇒ **Select the LTQ_DEMO "Search Tasks" option on the left side**

This opens the page listing the searches performed on this instrument. Searches still running will be highlighted in green.

[List Search Results by Folder]
Total : 513 (11 Pages) 1 2 3 4 5 6 7 8 9 10 11

Task ID	Analyst PlateID	Project	Task Name	Status	Task Detail	Result Detail
578		32	yst search The task was set to run. But it is not running. Click task detail to stop it or run it again.	Error		
579		32	se test	In task queue		
577		32	queue gpm	Finished		
576		32	queue	Stopped by Frank Liu		
575		32	large file mml	Finished		
574		32	cluster test	Finished		

Other important status information can also be obtained in Search Tasks view. While green indicates a file being actively searched, a blue colour indicates that a sample is currently in the queue. Yellow highlights an error with the search. No other searches can be initiated until this problem is resolved, either through successful running of the problematic search, or by stopping the task.

IMPORTANT: If an error is encountered while tasks are in the queue, one of these tasks must be manually re-started (the other Tasks will then be searched in queue).

⇒ **Clicking on the Task Detail icon in the column will open up the same status page as above.**

⇒ **To obtain the results, click on the "Result Detail" icon at the extreme right of the table.**

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LTQ_DEMO Search Tasks

Project Name ID
Demo Yeast Gel 1
Demo Yeast Gel Free 2
Demo Human Gel Free 3

[List Search Results by Folder]
Total : 4 (1 Page) 1

Task ID	Analyst PlateID	Project	Task Name	Status	Task Detail	Result Detail
7	1	1	Gel_based demo search	Finished		
6	0	2	yeast_demo_search	Finished		
5		3	Demo_human	Finished		
1	1	1	demo seach	Finished		

LTQ_DEMO Search Tasks

LTQ_DEMO New Task

LTQ_DEMO Task Finder

Running Task Status

View Search Log

View TPP Log

View Parser Log

View Search Results

⇒ Select the "Result Detail" for one search task

This opens up a new page.


The search results are displayed at the bottom of the page. The blue link will connect to the search engine page.

Note that if using the Demo sites from external computers, you will not be able to view the results from the search engines (firewall protection).

This page also provides you with

- 1) list of the other Task IDs associated with this folder
- 2) the option of analyzing your search results using the TPP (either for single files or for merged files)
- 3) the possibility to link files to the Analyst module
- 4) the file parsing tool that allow you to transfer your search results to the Analyst module.

LTQ_DEMO Search Results

Task ID:	5	
Task Name:	Demo_human	
Folder ID	Folder Name	Project
21	 Demo_Human_GelFree_P3 0(MB)	Demo Human Gel Free

Status: Finished
 Start Time: 2010-01-07 19:50:19
 Set By: Prohits Administrator

Task ID	Task Name	Search Engine	Schedule	Status
5	Demo_human	Mascot=demo_human; GPM=human	Now	Finished
4	Demo_human	Mascot=Yeast;GPM=YST	Now	Stopped by Prohits Administrator

Set Search Results to Run TPP

[\[New \]](#)

TPP ID	TPP Name	Parameter Set	Status	Set By
3 [log]	demo1	unlabeled	Finished	Prohits Administrator

Parse Hits to Prohits Analyst database

[\[Detail \]](#)

Parse Hits Status:	not saved
Parsed By:	

Reload

File ID	[Folder ID] / File Name	Size(KB)	Search Results	TPP
22	[21] / 8_MEPCE_pelletA.RAW	167,540	GPM	pepXML protXML
23	[21] / 9_MEPCE_pelletB.RAW	180,071	GPM	pepXML protXML
24	[21] / 10_EIF4A2_pelletC.RAW	183,275	GPM	pepXML protXML
25	[21] / 11_EIF4A2_pelletD.RAW	132,643	GPM	pepXML protXML

Running the TPP after completion of searches and merging samples prior to TPP analysis

To add new results files to be analyzed with the TPP to an existing TPP task, click



icon in the "Status" column of the box [Set Search Results to Run TPP]. You can simply click on the boxes in the TPP column of the results tables. When desired files are selected, press [Run TPP]. To create a completely new TPP task (e.g. if the TPP parameters have changed), click [New], select desired parameter set and desired files and press [Run TPP].

Set Search Results to Run TPP [\[New \]](#)

TPP ID	TPP Name	Parameter Set	Status	Set By
5 [log]	demo	unlabeled	Finished	Prohits Administrator
		<input type="text"/> Edit		

Merges together search result files --- [\[Select Files \]](#)

There are cases where you may want to merge files prior to running the TPP (examples include fractionated samples, gel-based or otherwise). This is a simple process in ProHits. The two requirements are that the searches be performed using the same search engine (Mascot and X!Tandem files cannot be combined) and that the results are located within the same Search Task folder. Select the "Merge" option and the files to be combined.

Selecting the "Merge" option will create a new entry at the bottom of the page. The TPP can be run on this entry in the same fashion as on individual files, by selecting the desired parameters and pressing "Run TPP".

At this point, we have performed database searching and have obtained results directly from the search engines, as well as results from the TPP pipeline. We are now ready to transfer these search results into the "Analyst" module.

The transfer involves two steps: 1) linking the initial file to an entry created in the Analyst module; and 2) parsing the search results.

Linking files to Analyst

⇒ link the file

You may have already linked the native file (not searched) to the Analyst modules through the "Storage" area. If so, the "link" icon by the file size will be coloured.

The screenshot displays the 'LTQACG Search Results' interface. It includes a sidebar with navigation links like 'Home', 'Storage', 'Auto Search', 'Help', 'Analyst', and 'Logout'. The main content area shows details for Task ID 107, including its name 'test_TPP', folder ID 317, and project 'Gingras_Lab_Public'. Below this, there's a table of tasks and a section for 'Set Search Results to Run TPP'. At the bottom, a table lists search results with columns for File ID, Folder ID / File Name, Size (KB), Search Results, and TPP. A white link icon is visible next to the file size in the search results table.

Task ID	Task Name	Search Engine	Schedule	Status
200	for demo	Mascot=flag_RefSeq	Now	Finished
107	test_TPP	Mascot=flag_RefSeq;GPM=GPM_RefSeq1	Now	Finished
24	sike	Mascot=acg_IPI	Now	Finished

TPP ID	TPP Name	Parameter Set	Status	Set By
1 [log]	test	Gingras_MML	Finished	Anne-Claude Gingras


File ID	[Folder ID] / File Name	Size(KB)	Search Results	TPP
320	[317] / F_PPP2CAwt17_a_20071112.RAW	136,475	GPM	
320	[317] / F_PPP2CAwt17_a_20071112.RAW	136,475	Mascot	pepXML protXML

A white link  indicates that no link has been established at this point, as in the example above.

See page 6 for details about manual and automatic link creation.

Parsing files to the Analyst module

You are now ready for parsing (transferring results to the Analyst module), as you have a linked file

() and search results. In this case you also have TPP results. Both types of results can be parsed.

⇒ **Select the “Detail” link in the parsing area**

Parse Hits to Prohits Analyst database
[\[Detail \]](#)

Parse Hits Status: not saved

Parsed By:

Pre-defined Filter Set: default [\[Save As\]](#)

Parse Results from ☐ GPM/Mascot ☐ TPP ☒ Both GPM/Mascot and TPP

Mascot

Ions score cut-off <:

Require bold red peptide : ☒

Save Protein Score > save all hits

Max. number of hits :

Significance threshold p <:

GPM

Ions expect log(e) cut-off > -1 0

Save Protein expect log(e) < -1 0









TPP

TPP_PARSE_MIN_PROBABILITY = 0.05

Run

Reset

Reload

File ID	[Folder ID] / File Name	Size(KB)	Search Results ▼ select all <input checked="" type="checkbox"/>	TPP select all <input checked="" type="checkbox"/>
22	[21] / 8_MEPCPE_pelletA.RAW	167,540 	GPM  <input checked="" type="checkbox"/>	pepXML  protXML  <input checked="" type="checkbox"/>
23	[21] / 9_MEPCPE_pelletB.RAW	180,071 	GPM  <input checked="" type="checkbox"/>	pepXML  protXML  <input checked="" type="checkbox"/>

You can transfer (parse) results from the search engines (GPM/Mascot), from the TPP or both. You can select the parameters for the parsing cut-off for Mascot and X!Tandem/GPM search engines. For the TPP, all hits with a probability greater than the cut-off selected by the administrator in the Prohits configuration file (we are using $P > 0.05$) are automatically parsed. Check the [select all] box at the top of the appropriate column or manually select files to be transferred to the Analyst module.

⇒ **Press “Run” to initiate parsing**

The “processing” status notification will appear.

When parsing is successfully completed, a green check mark will appear.

Parse Hits to Prohits Analyst database [\[Detail \]](#)

Parse Hits Status: not saved

Parsed By:

Pre-defined Filter Set: default [\[Save As \]](#)

Parse Results from ☐ GPM/Mascot ☐ TPP ☒ Both GPM/Mascot and TPP

Mascot

ions score cut-off <: 35

Require bold red peptide : ☒

Save Protein Score > save all hits

Max. number of hits : 500

Significance threshold p <:

GPM

ions expect log(e) cut-off > -1 0

Save Protein expect log(e) < -1 0

TPP TPP_PARSE_MIN_PROBABILITY = 0.05

[Run](#) [Reset](#)

[Reload](#)

File ID	[Folder ID] / File Name	Size(KB)	Search Results	TPP
			select all <input checked="" type="checkbox"/>	select all <input checked="" type="checkbox"/>
22	[21] / 8_MEPCE_pelletA.RAW	167,540	GPM	pepXML protXML <input checked="" type="checkbox"/>
23	[21] / 9_MEPCE_pelletB.RAW	180,071	GPM	pepXML protXML <input checked="" type="checkbox"/>
24	[21] / 10_EIF4A2_pelletC.RAW	183,275	GPM	pepXML protXML <input checked="" type="checkbox"/>

In the event that you decide to link or parse different file(s) to the same Analyst entry, you can remove the parsed files or the link: Alongside the tick box, the icon can be selected if you want to remove the hits from the Analyst module. Note that you can also unlink a sample by clicking on the or and selecting "remove link".

Parse Hits to Prohits Analyst database [\[Detail \]](#)

Parse Hits Status: Completed 2010-01-13 11:01:36

Parsed By: Prohits Administrator [\[Detail \]](#)

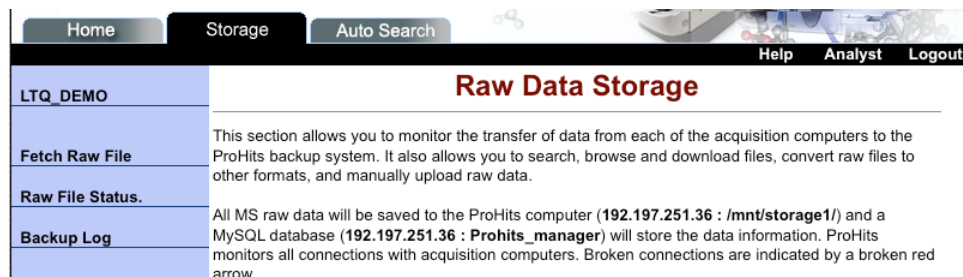
[Reload](#)

File ID	[Folder ID] / File Name	Size(KB)	Search Results	TPP
22	[21] / 8_MEPCE_pelletA.RAW	167,540	GPM	pepXML protXML
23	[21] / 9_MEPCE_pelletB.RAW	180,071	GPM	pepXML protXML
24	[21] / 10_EIF4A2_pelletC.RAW	183,275	GPM	pepXML protXML

Other options

You have now completed the basic tour of the Data Management module. The following few pages will explore a few other options within the Data Management module: 1) Creating activity reports; 2) Searching ("fetching") files; 3) Basic troubleshooting of the Data Management module.

The first few options are accessed from the "Storage" page:



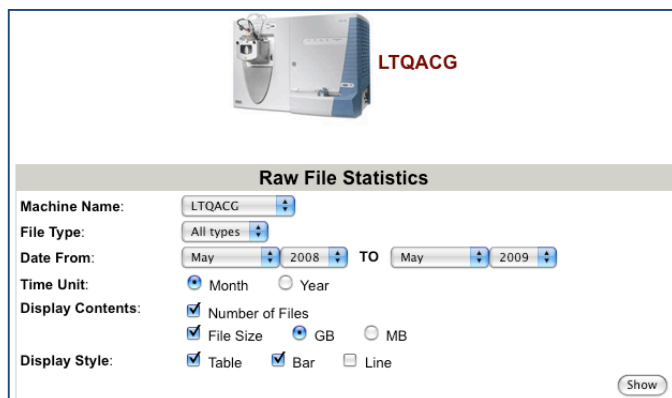
Creating activity reports for the RAW files

⇒ From the storage tab, select the "Raw File Status" option

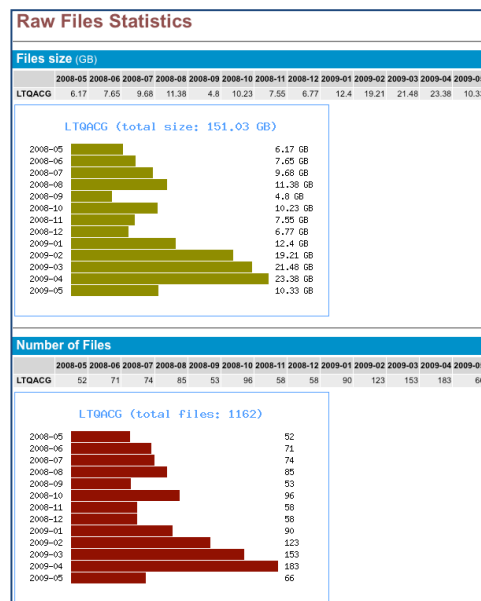
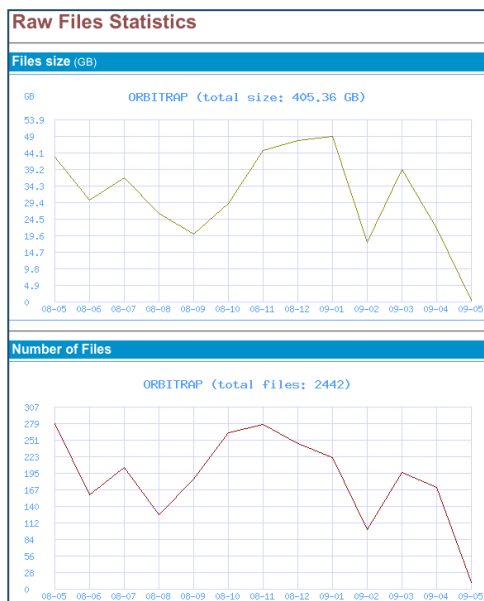
This opens up a new window (here we are simply showing one of the SLRI instruments as an example).

⇒ Select the instrument you want the report on, the dates of the report and time units, as well as the contents and style of the display

You could also choose to get the report for all instruments linked to ProHits.





⇒ Press "show" to visualize selected display

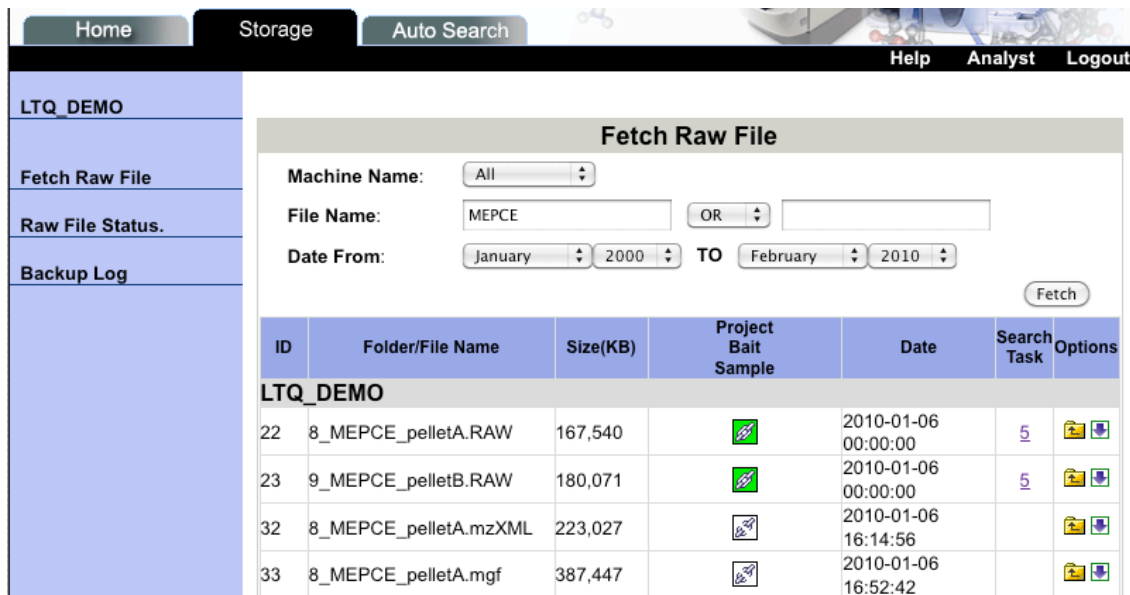














Searching files and retrieving RAW data

⇒ Select “Fetch Raw File”

This will open a new window. Select the desired instrument (or all instruments), dates if applicable, as well as keywords that are part of the file name (note that you can perform logical operations). Press [Fetch] to retrieve results.

The “Options” in the last column allow you to download the data (.RAW , .mzXML or .mgf) onto your computer () , and to open the parent folder ().



ID	Folder/File Name	Size(KB)	Project Bait Sample	Date	Search Task	Options
LTQ_DEMO						
22	8_MEPCE_pelletA.RAW	167,540		2010-01-06 00:00:00	5	 
23	9_MEPCE_pelletB.RAW	180,071		2010-01-06 00:00:00	5	 
32	8_MEPCE_pelletA.mzXML	223,027		2010-01-06 16:14:56		 
33	8_MEPCE_pelletA.mgf	387,447		2010-01-06 16:52:42		 

⇒ To retrieve the searched results, you can click the search task number in the “Search Task” column.

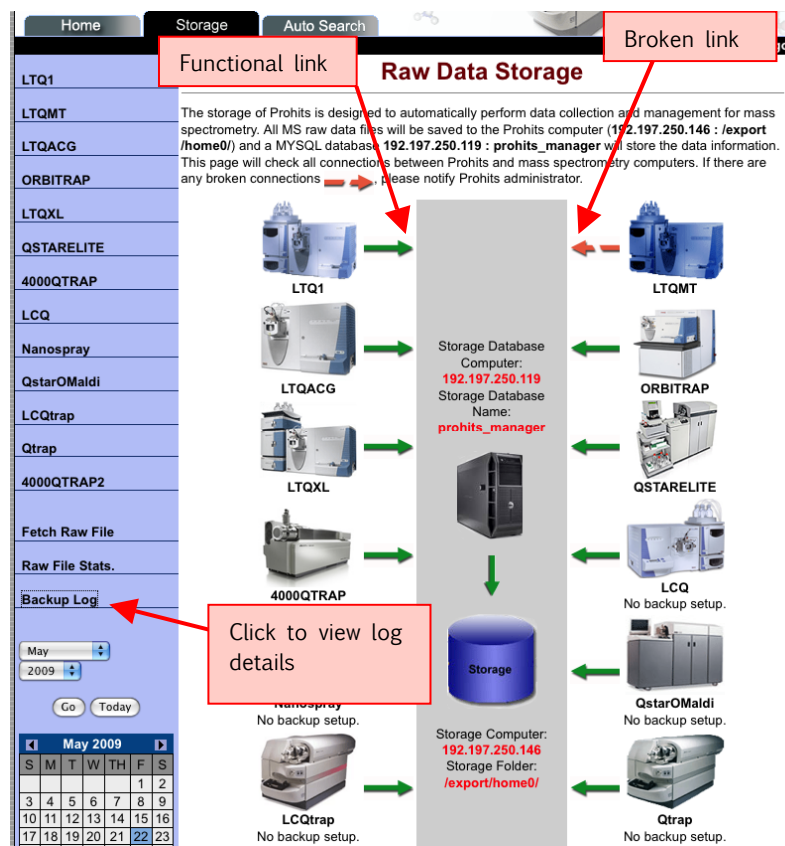
Basic Troubleshooting of the Data Management module

ProHits Data Management requires a connection between all of your acquisition computers, the search engine computers(s) and the storage computer. To facilitate the detection of broken links between these computers, ProHits has implemented an easy visual guide, both in the storage and auto search modules.

⇒ From the Data Management entry page, select the "Storage" tab

As before, all of the instruments in the facility are listed. The green arrows indicate that the connection between each instrument and the storage areas is functional. If an automated backup has been selected, this also indicates that the backup was performed on schedule. Note that there is a broken connection between one of the instruments and the storage computer, easily identified by a broken orange arrow (in this case, the computer was offline for maintenance). Notify the ProHits administrator when you detect such arrows.

⇒ Click on the "Backup" log (left side of the screen, toward bottom) to monitor the transfer of data from the acquisition computers to the storage computers and read any error messages



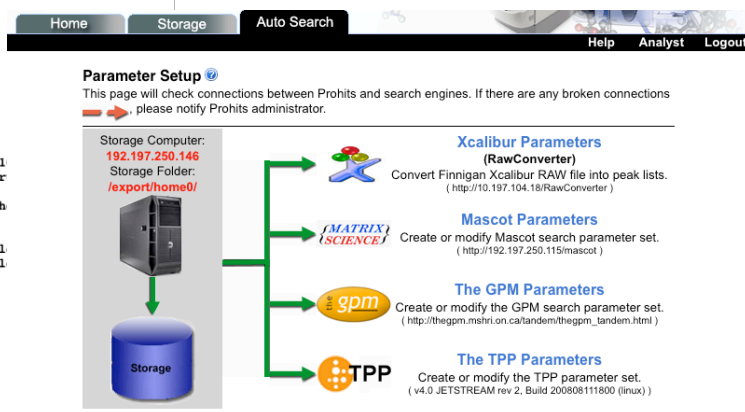
Log File 'raw_back.log'

Display last : 100 lines

```

10089 end of QSTARELITE 2009-05-22 8:04:27
10088 copied 6: /mnt/QSTARELITE/1_AJ/2009_05_20_Grb2_iTRAQ_op/Data
10087 process QSTARELITE 2009-05-22 8:03:36
10086 Backup QSTARELITE start at 2009-05-22 8:03:36
10085 PSID:3771 QSTARELITE
10084 end of 4000QTRAP2 2009-05-21 23:07:01
10083 copied 2: /mnt/4000QTRAP2/Andrew_J/2009_05_20/Data
10082 copied 1: /mnt/4000QTRAP2/Andrew_J/2009_05_20/Batch
10081 process 4000QTRAP2 2009-05-21 23:07:00
10080 end of 4000QTRAP 2009-05-21 23:07:00
10079 copy 6: /mnt/4000QTRAP/CJ_Yong/2009_05_07_0430ShcA/Data/0430ShcA_R_21
10078 copied 20: /mnt/4000QTRAP/CJ_Yong/2009_05_07_0430ShcA/Data/0430ShcA_r
10077 copied 1: /mnt/4000QTRAP/CJ_Yong/2009_05_07_0430ShcA/Batch
10076 copied 1: /mnt/4000QTRAP/CJ_Yong/2009_05_07_0430ShcA/Acquisition Meth
10075 process 4000QTRAP 2009-05-21 23:06:51
10074 end of QSTARELITE 2009-05-21 23:06:51
10073 copy 0: /mnt/QSTARELITE/Tempo Method Maker/Project Information/event1
10072 copy 1: /mnt/QSTARELITE/Tempo Method Maker/Project Information/event1
10071 copy 1: /mnt/QSTARELITE/Tempo Method Maker/BioAnalyst
10070 copied 10: /mnt/QSTARELITE/1_AJ/2009_05_20_Grb2_iTRAQ_op/Data
10069 copied 2: /mnt/QSTARELITE/1_AJ/2009_05_20_Grb2_iTRAQ_op/Batch
10068 process QSTARELITE 2009-05-21 23:05:15
10067 end of LTQXL 2009-05-21 23:05:15
10066 copied 1: /mnt/LTQXL/Yasmina_P36
10065 process LTQXL 2009-05-21 23:05:05
10064 end of ORBITRAP 2009-05-21 23:05:05
10063 copied 10: /mnt/ORBITRAP/Fall08dev
10062 copied 1: /mnt/ORBITRAP/EK Install Data
10061 process ORBITRAP 2009-05-21 23:04:27
10060 end of LTQACG 2009-05-21 23:04:27
10059 copied 3: /mnt/LTQACG/MM_IP_LCMS
10058 process LTQACG 2009-05-21 23:04:01
10057 end of LTQMT 2009-05-21 23:04:01
10056 process LTQMT 2009-05-21 23:04:01

```



The same visual display and log details are also found in the AutoSearch module.